Original Research Article

Investigation of the interaction of drug tetradecyltrimethylammonium bromide with cetyltrimethylammonium bromide at different temperature

Abstract

Antibiotic interaction between tetradecyltrimethylammonium bromide (TTAB) with cetyltrimethylammonium bromide (CTAB) has been done in solution and within the attendance of salts at several temperatures (298.15, 303.15, 308.15, 313.15 and 318.15 K). Onecritical micelle concentration (CMC) was noted for pure CTAB and their mixture with the drug tetradecyltrimethylammonium bromide (TTAB). The CMC values for mixed systems (TTAB + CTAB) within the presence of salt exhibited lower in magnitude as compared to their absence. This acknowledged the first micellization of the mixture of TTAB and CTAB. All the G^0m values were found to be negative for all systems. The H^0m and S^0m values disclosed that hydrophobic and electrostatic interactions were increasedwithin the presence of salts compared to their absence at lower and better temperatures respectively. The opposite thermodynamics parameters like transfer energy (G^0m.tr.), transfer enthalpy (H^0m.tr.) also as transfer entropy (S^0m.tr.) were also determined and discussed intimately. The inherent enthalpy gain (H0, m) and therefore the compensation temperature (Tc) were also estimated and deliberated. Molecular dynamics simulation exposes that aqueous also as salt environment have an impact on the hydrophobic interaction between tetradecyltrimethylammonium bromide (TTAB) with cetyltrimethylammonium bromide (CTAB).

Keywords: TTAB, CTAB and CMC.

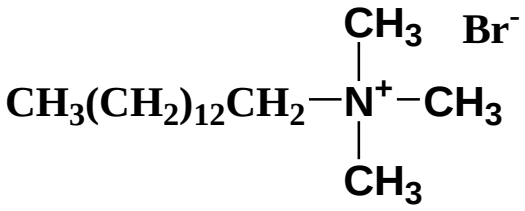
1. Introduction

The existence of both hydrophobic, also as hydrophilic parts in a surfactant is responsibleto make aggregates in aqueous/ nonaqueous solution, termed as micelles and this phenomenon takes place elsewherea particular surfactant concentration which is acknowledged as critical micelle concentration (CMC) [1–3]. The micelles of surfactant are employed as a model of biological membranes. Appliances of surfactants are mainly hooked into the complex formation behaviour of surfactants with solutes like drugs, dyes, organic molecules etc. [1–7]. In pharmaceutical industries, micelles are ready to solubilize the feebly soluble organic compounds in solution by integrating them within the micellar phase [8-9]. Micelles have large surface area; therefore, they're suitably exploited to perform as catalysts for varied chemical reactions, ready to modify the reactions pathways, rates also as equilibria [8-9].

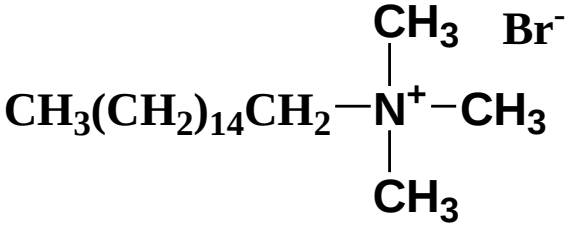
Moreover, it's usually employed to cure pneumonia, tract illness, and abdominal infections alongsidethose opposing to other antibiotics and prostatitis. On the opposite hand, among an outsized number of conventional surfactant, we've chosen the cationic surfactant CTAB which have multipurpose uses like removal ability of heavy metal from magnetic nanoparticles [5] and use as an adsorbent to re-move of toxic and harmful compounds like herbicides from the water. Although literature surveys show the presence of an outsized

number of studies on the mixed surfactant systems, to the simplest of our knowledge a detailed study on the mixed micelle formation between tetradecyltrimethylammonium bromide (TTAB) and cetyltrimethylammonium bromide (CTAB) (Schemes 1 and 2) has not been yet studied. Considering these views during this study different micellar parameters like CMC, the ideal value of the critical micelle concentration, micellar mole fractions and their ideal values, activity coefficients, degree of dissociation (g) also as different thermodynamic parameters (standard free energy change ($G^{o}m$), standard enthalpy change ($H^{0}m$), standard entropy change ($S^{0}m$) of micellization also as the excess free energy of micellization are determined from conductivity technique and theoretical calculations to explore the interactions between the components present in mixtures.

Even though, a numerous investigation on the surfactants interaction through various molecules alongside drugs is accounted for earlier [3–6, 10–17]. But to the simplest of our consciousness, just some is acknowledged on the interaction of TTAB (drug) utilizing CTAB using the conductometric method. The study is of potential significance to realize in-sight into complex aggregation behaviour of surfactant with drug both in absence and presence of salts. Furthermore, this study demonstrates that while designing such formulations one must consider the associated physicochemical changes which can affect the pharmacokinetic activity of medicine and therefore the delivery properties of these formulations. In our earlier studies, the interaction of medicine with ionic surfactants in absence also as in the absence of various salts was accounted [14–18].



Scheme1. Molecular structure of tetradecyltrimethylammonium bromide (TTAB)



Scheme2. Molecular structure of cetyltrimethylammonium bromide (CTAB)

In this study, the interaction of TTAB through CTAB (cationic surfactant) in the absence and presence of NaCl, KCl, and NH4Cl was investigated via a conductometric method. The utilization of additives like inorganic salts, drugs etc.maybe a familiar process to switch the micellization performance of amphiphiles. The existence of salts in amphiphiles lessens the electrostatic repulsion among the charged head group which drops the critical micelle concentration (CMC). Additionally, strong electrostatic interactions significantly influence the adsorption of amphiphile molecules at the interface of air and water [19,20]. Hence, it is often assumed that the degree of adsorption within the presence of salts should be considerably different as compared to their absence within the surfactant solution. the varied parameters like critical micelle concentration (CMC), counter ion binding (β), thermodynamic parameters (G0m, H0m, and S0m) related with the TTAB and CTAB

interaction in solution and presence of salts are estimated for instance the interaction behaviour between TTAB and CTAB.

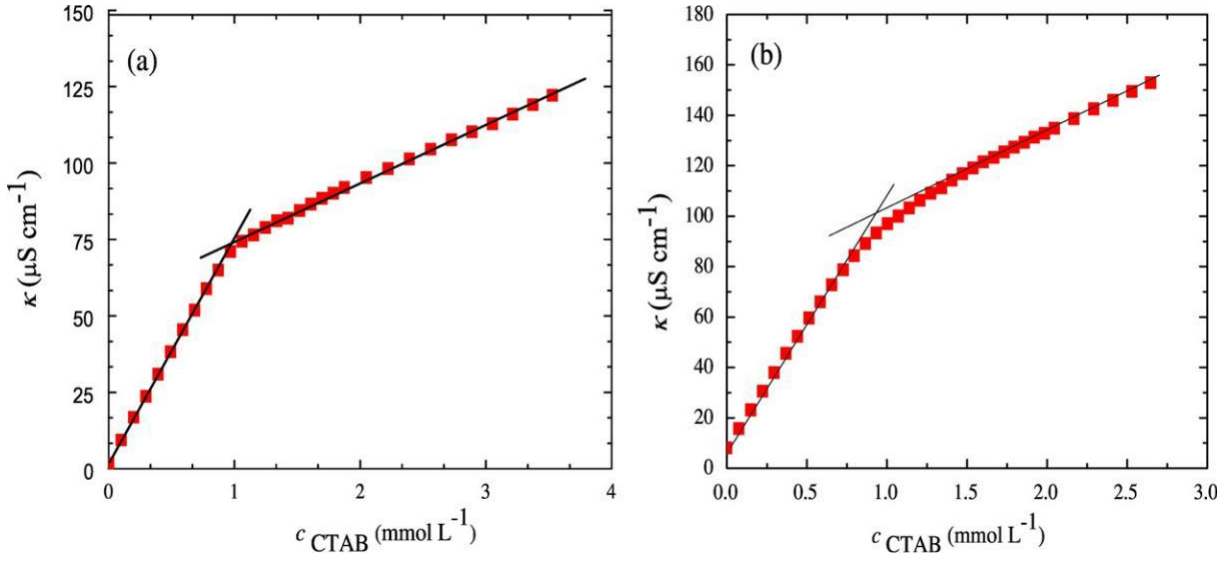


Fig.1. Specific conductance versus concentration of CTAB for (a) pure CTAB in water and (b) (TTAB + CTAB) mixed system in water containing 1.032 mmol L^{-1}TTAB at 303.15 K.

2. Experimental Section

2.1. Preparation of Solutions

The stock solutions of TTAB (drug) and surfactant (absence or presence of a known concentration of NaCl, KCl, NH_4Cl) were prepared using double de-ionized distilled water having the specific conductivity in the range of 1.5–2 μS/cm. All the materials working in the present study were used without further purification. Cetyltrimethylammonium bromide CTAB was purchased from Aldrich, USA. TTAB as USP standard sample NaCl, KCl and NH_4Cl was used in this study.

2.2. Conductivity Technique

An aqueous solution 25 mmol/L CTAB prepared in water or (TTAB+ water), in absence or presence a known concentration of NaCl, KCl, NH_4Cl; is gradually added to 20 mL of water or (TTAB + water) solution of a particular drug (TTAB) concentration (absence or presence a known concentration of NaCl, KCl, NH_4Cl) at a fixed temperature. After that, the specific conductance of the prepared mixtures was evaluated through a conductivity meter having a dip cell (a glass electrode) of cell constant 0.97 cm^{-1}[5–8,14–18,21,22]. This instrument was standardized using solutions of KCl of the appropriate range of concentration. An alternating current (AC) supplier at a frequency of 60 Hz was applied for conductance measurements. The accuracy of the conductance measurements is in a range of ±0.5%. The temperature of systems was controlled within the stated range by circulating water throughout the solution having the error of ± 0.2 K. To see the effect of salt, both the TTAB as well as CTAB

solutions are prepared in presence of NaCl, KCl, NH_4Cl, therefore, all the solutions hold the same concentration of salt.

2.3. Molecular Dynamics Simulations

Molecular dynamic (MD) simulation was performed on two systems containing surfactant-drug with water in the presence of salt and without salt. For surfactant, 32 molecules of CTAB were studied. The preliminary surfactant molecule was improved by Universal Force Field [23]in Gaussian 09 Software package [24]then each surfactant molecular are balancing and grouped through continuous minimization. Six drugs molecular are haphazardly placed in each system. For considering salt holding surfactant-drug system, 10 Na^+, and 10 Cl^- ions were added. All molecular dynamics simulations were lead using NOVA force field in the suite of YASARA Dynamic pro-gram [25,50]. A cut-off radius of 8.0 Å was retained for short-range van der Waals as well as Coulomb interactions. The particle-mesh Ewald method [26]was applied to calculate the long-range electrostatic interactions. Periodic boundary condition (cell box of 54 Å × 68 Å × 46 Å) and temperature of 298 °C were deliberated for all simulations. Timestep of 1 fs was used and simulation snapshots were kept at every 100 ps 2261 water molecules was added to retain the solvent density of 1 g/mL for both systems. Anaggregate of 17,008 atoms was present in those systems. The systems were minimized along with equilibrated with the default protocols of the YASARA dynamic. Lastly, 3 ns non-constrained MD simulation was implemented for all system.

3. Result and Discussion

3.1. Critical Micelle Concentration (CMC) & Counter ion binding (β)

In the current investigation, the values of critical micelle concentration (CMC) are evaluated by the observed change in specific conductance values versus the concentration of CTAB in water or TTAB and water mixture. Fig.1demonstrates the variation of specific conductance (κ) vs. concentration of surfactant (c_{CTAB}) of pure CTAB in aqueous solution or (TTAB + water) mixed system at 303.15 K. The conductivity value of solution changed linearly with the concentration of amphiphile in the pre and post-micellar regions. A clear breakpoint was presentedin the κ versus c_{CTAB}

Table1: Physiochemical parameters for CTAB and (TTAB+CTAB) system containing 1.032 mmol/L TTAB drug in aqueous solution within the attending of different salts of different concentrations at fixed and numerous temperatures

Systems	Medium	T (K)	C_{salts} (mmol/L)	CMC (mmol/L)	$X_{CMC} \times 10^5$	α	B
CTAB	H_2O	298.15	0.00	1.01	1.82	0.27	0.73
		303.15		0.99	1.78	0.28	0.72
		308.15		1.05	1.89	0.29	0.71
		313.15		1.16	2.09	0.30	0.70
		318.15		1.23	2.21	0.30	0.70
		323.15		1.33	2.39	0.31	0.69

(TTAB+ CTAB)	H_2O	298.15	0.00	0.95	1.71	0.31	0.69
		303.15	0.00	0.93	1.67	0.30	0.68
		308.15	0.00	1.00	1.80	0.34	0.66
		313.15	0.00	1.06	1.91	0.35	0.65
		318.15	0.00	1.16	2.09	0.37	0.63
(TTAB + CTAB)	H_2O	303.15	0.00	0.93	1.67	0.30	0.68
(TTAB + CTAB)	(NaCl + H_2O)	303.15	0.505	0.83	1.49	0.31	0.69
			1.067	0.70	1.35	0.29	0.71
			2.035	0.60	1.21	0.29	0.71
			3.013	0.60	1.08	0.28	0.72
(TTAB + CTAB)	(KCl + H_2O)	303.15	0.506	0.84	1.51	0.31	0.69
			1.078	0.77	1.39	0.31	0.69
			2.038	0.70	1.26	0.29	0.71
			3.087	0.64	1.15	0.28	0.72
(TTAB + CTAB)	(NH_4Cl+H_2O)	303.15	0.507	0.86	1.55	0.31	0.69
			1.035	0.80	1.44	0.32	0.68
			2.009	0.74	1.33	0.27	0.73
			3.003	0.68	1.22	0.26	0.74

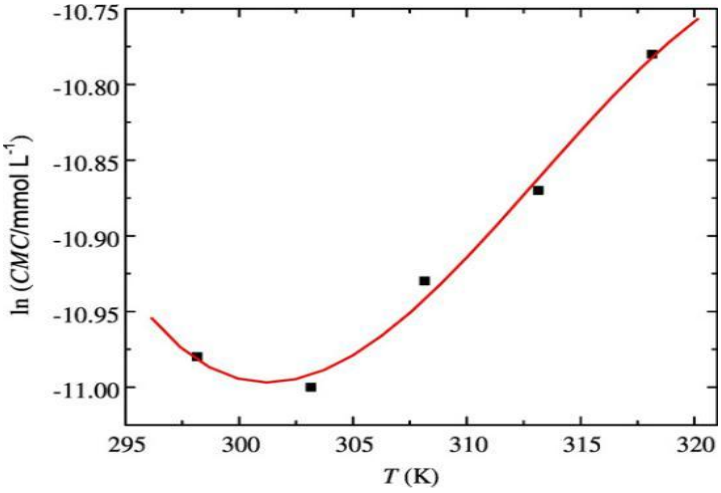


Fig.2. ln (CMC/mmol L^{-1}) versusTfor (TTAB + CTAB) mixed system in water.

The plot was attained in between pre and the post-micellar region is deemed as the critical micelle concentration (CMC) and it is equivalent to the concentration of amphiphile parallel to the breaking point [3,14–18,27,28].At low surfactant concentrations, the first rise of specificconductance values was owing to the associations of the free CTA^+ and Br^- ions. However, above the CMC, the rise of specific conductance values develops smaller due to the formation of CTAB micelles and also because of the condensation of the Br^- ions with CTAB micelles to shape the Helmholtz layer. This stabilizes the self-micellized amphiphiles using surface charge neutralization and hence dropping intermolecular repulsion potential [29]. Therefore the formed micelles have lessermobility compare to the free ions of CTAB. The literature exposed that the value of CMC of pure CTAB in the water at 303.15 K lies in the scale of 0.8–1.1 mmol/L which is in satisfactory agreement with our found values [4,8, 11, 18].

The degree of ionization (α) of micelles is assessed from the relation of the slopes of the pre and post-micellar regions correlated to the above and below CMC [4,14–18,21,22]. The CMC or X_{CMC} values for (TTAB+CTAB) mixed system in aqueous solution are lesser in magnitude in comparison to that of pure CTAB and the values of CMC reduce gradually with the increase of the concentrations of drug for (TTAB + surfactant) mixed system at 303.15 K. This demonstrates the interaction between TTAB and CTAB and reveals that the addition of TTAB in the solution supports the formation of CTAB micelle.

The values of CMC or X_{CMC}, α as well asβ for (TTAB + surfactant) mixture at 303.15 K in the attendance of salts are revealed in Table 1. The concentration of electrolytes in the body membranes may differwith time. The presence of various electrolytes and its concentration may influence the interaction propensity of surfactant. Hence, it is crucial to have an awareness of aggregation phenomena for pure CTAB and TTAB + CTAB mixtures utilizing temperature together within attendance of electrolytes. Herein, the values of CMC of (TTAB + CTAB) mixture at 303.15 K in the incidence of all the inorganic salt consumed in the present study are discovered to be lower in magnitude in comparison to the salt-free solution. The CMC value of pure CTAB and their mixtures with TTAB decreases in the presence of salt (Table 1). In the case of ionic surfactants like the inorganic salt added CMC decreases [4, 27, 28]. The values of CMC are also decreased with the enhancement of the ionic strength (concentration) of salts. This directs that a higher concentration of salts provides a convenient environment for micellization of our studied (TTAB + CTAB) system. The co-ions for pure as well as mixed system micelles are Na^+, K^+, and NH^+_4. The effect of salts on the decrease of CMC or X_{CMC} values of mixed systems followed the order: CMC_{NaCl}> CMC_{KCl}> CMC_{NH4Cl} (Table1). This displays that NaCl is more effective in the reduction ofCMCofthe current studied system in comparison to KCl and NH_4Cl. The variation of CMC values possibly owing to the attendance of different cations in the salts retaining identical anion (Cl^-). $NH^+_4$is the least effectual in lessening the CMC owing to the small size along with bulky hydrated radius. Therefore this salt executes as a water-structure promoter, lessening the accessibility of H_2O to the micelles. Analogousmanner of these cations on the CMC values of ionic surfactant has also been narratedbefore[4,50].

The values of CMC or X_{CMC}, α, and β for pure CTAB and (CFH + CTAB) mixed system at various temperatures in aqueous solution are shown in Table 1.

This behaviour of nonlinearity/minimum position in the CMC versus T plots is also found in the literature for various other ionic surfactants in aqueous solution or presence of different solutes [14]. The effect of temperature on the values of CMC can be clarified employing the mode of hydration close to the monomers of CTAB and the TTAB arbitrated micelles of CTAB. At low concentration of surfactant the monomeric form the hydrophobic, as well as hydrophilic hydrations, are reasonable, while only hydrophilic hydration is feasible for accumulated CTAB. All kinds of hydrations are supposed to be reduced through the rise of temperature. A diminish in the hydrophilic hydration stimulates the micelle formation whereas the reduction of hydrophobic dehydration utilizing the uprising of temperature lined the formation of micelle [4,15]. Therefore, the extent of both features decides whether the values of CMC increase or decrease at a particular range of temperatures. Usually, the first

factor controls at a lesser temperature scale and after acertaintemperature, the second factor starts governing.

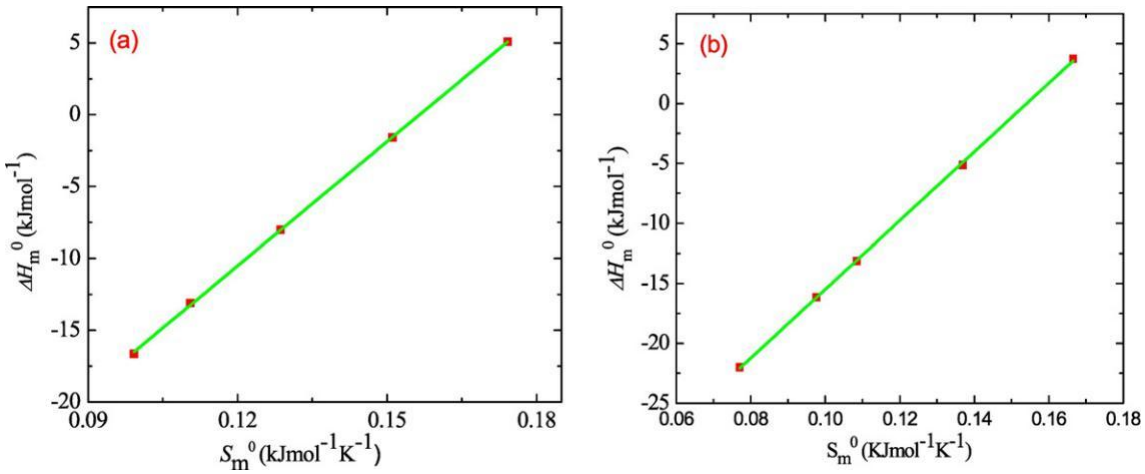


Fig.3. Enthalpy-entropy compensation plot for (a) CTAB in H_2O and (b) (TTAB + CTAB) mixed system in aqueous medium.

In the above mentioning equation, CMC values are in the applied in mole fraction unit. ln(CMC) versus T plot (Fig. 2) is achieved to be nonlinear. The plots are employed to evaluate H^0_m and slopes are represented at every studied temperature that is deemed as equivalent to $\partial \ln(CMC) / \partial T$ [15,25,28].

By increasing the drug concentration in the mixtures of TTAB and CTAB, G^0_m is found to be gradually extra negative. This suggests that in the mixed systems micelle formation take place easily together with the process of micellization is more spontaneous for drug-CTAB mixtures than CTAB alone. In attendance of salt, the negative G^0_m values are gained to be more negative indicatingthe encouraging association facts, whereas dynamic force for aggregation is considerably increased in the presence of NaCl/ KCl/ NH_4Cl. The H^0_m values for TTAB + CTAB mixtures in aqueous solution are found to be positive at 298.15 K, however, at a higher temperature, these values become negative and increased with the increase in temperature in the nonattendance and attendance of salt.

The S^0_m values are found to be positive at all temperature and their value decreases with an increase of temperatures. Therefore S^0_m and H^0_m values show the aggregation phenomenon is entropically controlled at lower temperatures while it turns into entropy as well as enthalpy controlled at higher temperatures. The negative values of H^0_m and positive S^0_m values for TTAB-surfactant mixed systems signify that besides hydrophobic, electrostatic interactions also take part a crucial role in the association of TTAB. This occurs using surfactant during the formation of TTAB supported surfactant micelles at higher temperature [34]. The hydrophobic involvement reduces whereas the electrostatic interaction enhances utilizing the rise of temperature, keeping the negative values of G^0_m almost constant at every temperature employed in the present study. Similar behaviour of H^0_m is also obtained for numerous ionic surfactants earlier [35,36]. Nusselder and Engberts [37]suggested that it is the London-dispersion forces that are liable in the micellar progression for the negative enthalpy values. The positive values of H^0_m ata lesser temperature are probably owing to the destruction of

arranged water molecules in the region of hydrophobic fractionsshowing the significance of hydrophobic interactions in the incident of micelle formation. In the case of both singleas well as the mixed system, positive togetherthe negative enthalpy values are also previously stated[38–41].

Upon addition of salt in the solution, the negative H^0_m values of (drug + CTAB) mixtures increased compared to the aqueous medium at higher temperatures. This designates that enthalpy contribution on the micellization of (drug + surfactant) mixtures is increased in the attendance of salts as competed to in the aqueous solution. The value of S^0_m for pure CTAB and TTAB + CTAB mixtures are attained positive at every considered temperature in the deficiency and occurrence of salt. However, their value decreases through the increase in temperature and the decrease of S^0_m value are due to depressing of hydration of hydrophobic parts of amphiphiles. The magnitude of the positive values of S^0_m for (TTAB+CTAB) mixed systems in the attendance of salt is more in comparison to the aqueous system at the lowest temperature. The positive values are obtained to be increased employing the enhancement of the salts concentration. The positive values of S^0_m can be explicated by the rupturing of iceberg structures adjoining the hydrophobic portions of surfactant monomer attended by the increased randomness in the core of the micelles[42]. At greater temperature, the values of S^0_m become lower in the presence of salt in the aqueous solution. Also at lower temperatures, the positive values of H^0_m are noticed to be increased with the increase of the concentrations of salts. In presence of salts, the higher positive values of both S^0_m and H^0_m at lesser temperatures are a good indication of increased hydrophobic interactions between the hydrophobic chains of surfactant and interface between the hydrophobic group of drug and CTAB. The higher negative values of H^0_m and relatively lesser positive S^0_m values at higher temperatures in the existence of salts also pointed out those electrostatic interactions are more important in the company of salts in contrast to the salt-free solution. Besides temperature, NaCl, KCl & NH_4Cl destroy hydrophobic hydration of surfactant monomers; therefore, much lower energy is required for aggregation in the incidence of salts.

In the mixed system of TTAB and CTAB in the aqueous solution, the contribution of G^0_m reduces along with that of entropy augmented using the rise of temperatures. In the presence of salt in the solution follow the more or less similar trend with few exceptions.

The negative values of $H^0_{m.tr.}$ are also accounted for the conveyance of salt and proteins from the aqueous system to a urea solution [45,46]. The negative value of $H^0_{m.tr.}$ pointed out that the move of the hydrophilic portion of CTAB from aqueous solution to the TTAB (drug), as well as TTAB and salt mixtures, is an exothermic manner while similar facts for the hydrophobic group is an endothermic phenomenon.

From all the system used in the present study, we get a linear line between the plots of H^0_m versus S^0_m with the regression coefficient (R^2) values in the range of 0.990–0.999 which is well-known as entropy-enthalpy compensation. Similar behaviour is also previously obtained by other researchers in aqueous solution [47]. The negative intercept is the intrinsic enthalpy gain ($H^{0,}_m$) and the slope of the compensation plots is the compensation temperature (T_c). The intercept H^0_m discloses the solute-solute interaction. It stalls for an indicator of the efficacy of the hydrophobic portion to denote to the micelle formation.

The T_c values for TTAB + CTAB mixture both in the nonattendance and attendance of salts are gained to be in the range of 286–302 K. The T_c values of any system in the range of 270–

300 K means this system can be engaged as an investigative test for the support of H_2O in the protein solution [48]. Therefore, the attained values of T_c in the current system are in satisfactoryconsistency with the normal values of T_c for the biological fluid. The more negative values of$H^{0,}{}_m$signify that the associationof surfactant, as well as drug-CTAB mixtures, are occurs even at $S^0{}_m = 0$. The raise of the negative values of $H^{0,}{}_m$ discloses the higher stability of the micelles formed in the solution.

4. Conclusions

This study illustrates the role of the variation of temperature as well as the concentration of the drug (levofloxacin hemihydrate) on the micellization phenomenon of cationic surfactant CTAB in absence as well as the attendance of salts. The addition of drug decreases the CMC value of pure surfactant at a different temperature. The decrease of the CMC of the mixture of CTAB with the drug in the presence of salts is also observed. The increase of the values of counter ion binding (β) with the gradual increase in the concentration of various electrolytes supports the stability of micelles. Molecular dynamics simulation disclosed the fact that in-deed salt environment promotes the micelle formation of the surfactant-drug complex compared to the no-salt environment. All values of $G^0{}_m$ are found to be negative in case of every studied system showing the formations of a micelle are spontaneous phenomena in a different medium. The values of $H^0{}_m$ and $S^0{}_m$ values reveal that hydrophobic and electrostatic interactions are enhanced in the presence of salts compared to those in the water at lower and higher temperatures respectively. From Molecular dynamics simulation, the subsequentremarks are obtained:

- salt promotes the micelle formation
- micelle adopts the nearly spherical shape
- drugs interact with the outer-sphere of the micelle closed to the cationic head and
- Micelle structure stays compressed over the simulation time.

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